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catena-Poly[[[tetraaquamagnesium(II)]-μ-glycine-κ^2O:O'] dinitrate]

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Key indicators

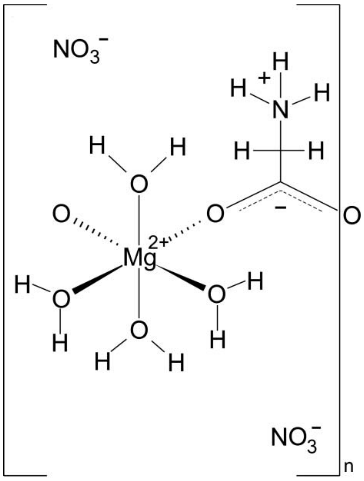
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.104
Data-to-parameter ratio = 18.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $\{[Mg(C_2H_5NO_2)(H_2O)_4](NO_3)_2\}_n$, contains *cis*-$MgO_2(H_2O)_4$ octahedra, which are connected by the glycine molecules to form helical chains. It is isostructural with its cobalt and nickel analogues.

Comment

In the course of our studies of new compounds of glycine with inorganic salts (Fleck & Bohatý, 2004, 2005*a*), we have investigated the family of glycine divalent metal nitrates. So far, only a few members of this group have been described in the literature. Here, we present the synthesis and structure of the title compound, (I) (Fig. 1). This magnesium salt is isostructural with its nickel (described in the following paper; Fleck & Bohatý, 2005*b*) and cobalt (Clegg *et al.*, 1987) analogues.



(I)

The main structural element in (I) is the coordination polyhedron of the metal cation. The Mg^{II} cation is coordinated by six O atoms (Table 1), forming a slightly distorted octahedron. Four of these O atoms belong to water molecules and two, in a *cis* configuration, belong to the carboxylate groups of glycine molecules.

The octahedra are connected *via* bridging glycine molecules, forming helical chains along the screw axes parallel to [010] (Fig. 2). Since the structure is centrosymmetric, both left-handed and right-handed helices occur. The N-terminal ends of the glycine molecules face away from the chain axis and form N—H$\cdots$O hydrogen bonds to the O atoms of the nitrate anions. Neither of the two crystallographically distinct nitrate groups coordinates to the cations; they are both located in the interstices between the chains. Their O atoms act as acceptors

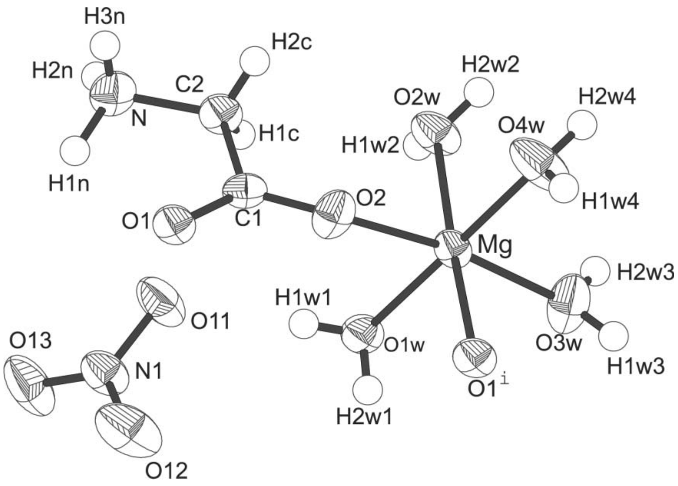


Figure 1
The atomic connectivity in (I), shown with displacement ellipsoids at the 50% probability level. [Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.]

for virtually all the hydrogen bonds (Table 2) donated by the amino groups and the water molecules. Only one hydrogen bond, namely O1*W*—H2*W*1···O2, donates to an O atom of the carboxylate group.

As observed for most compounds of glycine with inorganic salts, the glycine molecules in (I) exist in their zwitterionic form, $[H_3N^+CH_2COO^-]$. This is the most common case for such salts, although glycinium or glycinate compounds can also occur, *e.g.* copper glycinate nitrate monohydrate (Davies *et al.*, 1992) or glycinium nitrate (Narayanan & Venkataraman, 1975). In (I), the glycine molecules are slightly twisted from a planar conformation, the O2—C1—C2—N3 torsion angle being 179.56 (1)°. This value is within the expected range; perfectly planar glycine molecules are very rare (*e.g.* glycine magnesium dichloride tetrahydrate; Fleck & Bohatý, 2005*a*). The C—O distances within the carboxylate group are identical at 1.251 (1) Å; this is to be expected because of the delocalization of the carboxylate π electrons.

Experimental

A stoichiometric mixture of glycine and magnesium nitrate was dissolved in water. The solution was slowly evaporated at a temperature of approximately 295 K over a period of several weeks, yielding colourless crystals of (I) up to 1 mm in size.

Crystal data

$[Mg(C_2H_5NO_2)(H_2O)_4](NO_3)_2$
$M_r = 295.46$
Monoclinic, $P2_1/n$
$a = 9.230$ (2) Å
$b = 6.779$ (1) Å
$c = 19.052$ (4) Å
$\beta = 96.57$ (3)°
$V = 1184.3$ (4) Å^3
$Z = 4$

$D_x = 1.646$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2806 reflections
$\theta = 4.9–29.4°$
$\mu = 0.22$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
$0.08 \times 0.05 \times 0.04$ mm

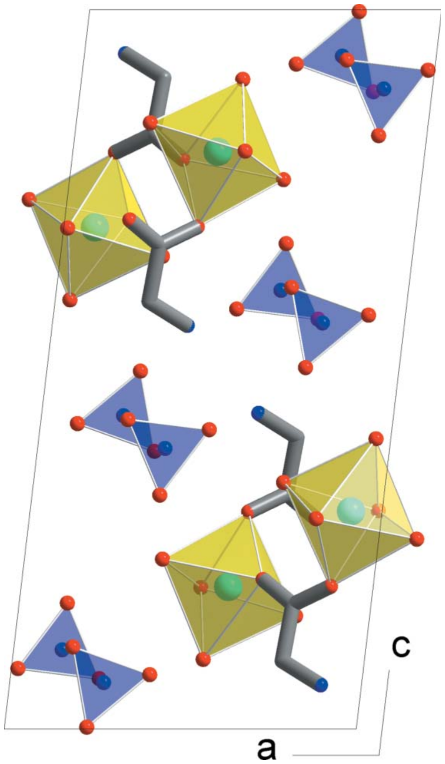


Figure 2
A packing diagram for (I), viewed along the helical chains parallel to [010]. The top left chain is right-handed and the bottom right chain is left-handed. Mg–O polyhedra are yellow, the NO_3 groups are blue, the glycine molecules are represented by a stick model, and H atoms have been omitted for clarity.

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*DENZO-SMN*; Otwinowski & Minor, 1997)
$T_{min} = 0.983$, $T_{max} = 0.991$
7524 measured reflections

3907 independent reflections
2918 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 31.5°$
$h = -13 \rightarrow 13$
$k = -9 \rightarrow 9$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.104$
$S = 1.02$
3907 reflections
216 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 0.27P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0077 (19)

Table 1
Selected geometric parameters (Å).

Mg1—O2*W*	2.0397 (10)	Mg1—O1	2.0688 (9)
Mg1—O4*W*	2.0447 (12)	Mg1—O3*W*	2.0764 (12)
Mg1—O2^i	2.0494 (10)	Mg1—O1*W*	2.1071 (11)

Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H1N···O23$^{\rm ii}$	0.90 (2)	2.11 (2)	2.9555 (19)	156 (2)
N—H2N···O11	0.87 (2)	2.05 (2)	2.9125 (16)	170 (2)
N—H3N···O22$^{\rm iii}$	0.79 (2)	2.33 (2)	3.0263 (18)	148 (2)
O1*W*—H1*W*1···O11$^{\rm iv}$	0.81 (2)	1.99 (2)	2.7833 (16)	168 (2)
O1*W*—H2*W*1···O2	0.80 (2)	2.02 (2)	2.7729 (13)	157 (2)
O2*W*—H1*W*2···O22$^{\rm v}$	0.73 (2)	2.13 (2)	2.8122 (17)	156 (2)
O2*W*—H2*W*2···O13$^{\rm vi}$	0.84 (2)	1.97 (2)	2.7958 (16)	170 (2)
O3*W*—H1*W*3···O12$^{\rm vii}$	0.82 (3)	2.02 (3)	2.8165 (16)	163 (2)
O3*W*—H2*W*3···O21	0.74 (2)	2.08 (2)	2.8099 (18)	166 (2)
O4*W*—H1*W*4···O23$^{\rm ii}$	0.80 (3)	2.05 (3)	2.8417 (17)	177 (2)
O4*W*—H2*W*4···O12$^{\rm vi}$	0.82 (3)	1.95 (3)	2.7732 (17)	178 (2)

Symmetry codes: (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (v) $-x+1, -y, -z$; (vi) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (vii) $-x+1, -y, -z+1$.

All H atoms were located in difference maps and freely refined.

Data collection: *COLLECT* (Nonius, 2003); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff *et al.*, 1996) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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